

Butylamine  
109-73-9 | DTXSID1021904

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -68.6 °C

Global applicability domain: Inside

Local applicability domain index: 8.40e-01

Confidence level: 6.65e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Butylamine</div> <div>Measured: -50.0</div> <div>Predicted: -68.6</div>	<div>Image not found</div> <div>Isobutylamine</div> <div>Measured: -85.0</div> <div>Predicted: -76.2</div>	<div>Image not found</div> <div>2-Butanamine</div> <div>Measured: -104</div> <div>Predicted: -82.6</div>
<div>Image not found</div> <div>Pentan-1-amine</div> <div>Measured: -55.0</div> <div>Predicted: -58.9</div>	<div>Image not found</div> <div>tert-Butylamine</div> <div>Measured: -72.7</div> <div>Predicted: -80.9</div>	